

Pentaerythritol  
115-77-5 | DTXSID2026943

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $2.96 \times 10^{-11}$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Inside

**Local applicability domain index:**  $5.45 \times 10^{-1}$

**Confidence level:**  $8.07 \times 10^{-1}$

## Nearest Neighbors from the Training Set

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2-(2-Ethoxyethoxy)ethanol

**Measured:**  $5.72 \times 10^{-11}$

**Predicted:**  $3.59 \times 10^{-11}$

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Propane, 1,1,3-trimethoxy-

**Measured:**  $1.92 \times 10^{-11}$

**Predicted:**  $2.33 \times 10^{-11}$

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Diethylene glycol

**Measured:**  $3.00 \times 10^{-11}$

**Predicted:**  $2.21 \times 10^{-11}$

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2-Amino-2-methylpropan-1-ol

**Measured:**  $2.80 \times 10^{-11}$

**Predicted:**  $2.88 \times 10^{-11}$

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3-Methoxybutan-1-ol

**Measured:**  $2.36 \times 10^{-11}$

**Predicted:**  $2.52 \times 10^{-11}$